XDS User's Guide

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1 FUNCTIONAL SPECIFICATION

The program package XDS [4, 5, 6] has been developed for the reduction of single-crystal diffraction data recorded on a planar detector by the rotation method using monochromatic X-rays. It includes a set of six programs:

• XDSTEMPLATE is a shell-script that copies an input template file to the directory from where xdstemplate was called. The templates are files containing preset values for various detector types. This makes it more convenient for the user to generate the correct input file required for running programs of the XDS package.

• XDS accepts a sequence of adjacent, nonoverlapping rotation images from a variety of imaging plate-, CCD-, and multiwire area detectors and produces a list of corrected integrated intensities of the reflections occurring in the images. The program assumes that each image covers the same positive amount of crystal rotation and that rotation axis, incident beam, and crystal intersect in one point, but otherwise imposes no limitations on detector position, or directions of rotation axis and incident beam, nor on the oscillation range covered by each image.

• XPLAN provides information to identify the optimal rotation range for collecting data. Based on detector position and unit cell orientation obtained from evaluating one or a few rotation images by XDS, it reports the expected completeness of the data by simulating measurements at various rotation ranges specified by the user, thereby taking into account already measured reflections.

• XSCALE places several data sets on a common scale, optionally merges them into one or several sets of unique reflections, and reports their completeness and quality of integrated intensities.

• VIEW displays rotation data images as well as control images produced by XDS. It is used for checking the correctness of data processing and for deriving suitable values for some of the input parameters required by XDS. This program was coded in the computer language C by Werner Gebhard in our institute. The other programs are written in FORTRAN 90, with the exception of a few C subroutines provided by Jan Pieter Abrahams (University of Leiden, The Netherlands) for handling compressed images.

• XDSCONV converts reflection data files as obtained from XDS or XSCALE into various formats required by software packages for crystal structure determination. The program allows to define test-reflections or to inherit reflections previously selected for monitoring the progress of structure refinement.

2 COMPONENTS OF THE PACKAGE

2.1 XDSTEMPLATE

The purpose of this little shell-script is to provide an appropriate input file required for running xds, xscale, or xdsconv. When calling xdstemplate, the user may request, for example XDS-ADSC.INP which serves as a template input file for processing images collected by the ADSC detector. This file is copied by xdstemplate to the current directory from where the command was issued. The user has to edit XDS-ADSC.INP to correctly describe the actual experimental conditions while many other parameter values usually remain untouched. After editing XDS-ADSC.INP, this file must be renamed into XDS.INP prior to invoking xds.

2.2 XDS

XDS is organized into 9 steps (major subroutines) which are called in succession by the main program. Information between the steps is exchanged by files (see Table 1), which allows repetition of selected steps with a different set of input parameters without rerunning the whole program. ASCII files can be inspected and modified by using a text editor, whereas types DIR and BIN indicate binary random access and unformatted sequential access files, respectively. All files have a fixed name defined by XDS, which makes it mandatory to process each data set in a newly created directory. Clearly, one should not run more than one XDS-job simultaneously in any given directory. Also, output files affected by rerunning selected steps (see Table 1) should first be given another name if their original contents are meant to be saved.

Data processing begins by copying an appropriate input file into the new directory, using the shell-script xdstemplate. Input file templates are provided with the XDS package for a number of frequently used data collection facilities. The copied input file must be renamed XDS.INP and edited to provide the correct parameter values for the actual data collection experiment. Since the length of file names is restricted in XDS to 50 characters it is recommended to abbreviate lengthy path names by a symbolic link, i.e. if the image directory resides on a different computer.

All parameters in XDS.INP are named by keywords containing an equal sign as the last character, and many of them will be mentioned here in context to clarify their meaning. Execution of XDS (JOB= XDS) invokes each of the 9 program steps as described below. Results and diagnostics from each step are saved in files with the extension .LP attached to the program step name. These files should always be studied carefully to see whether processing was satisfactory or – in case of failure – to find out what could have gone wrong.

XYCORR calculates a lookup table of additive spatial corrections at each detector pixel which is stored in the file XYCORR.TBL. Often, the data images are already corrected for geometrical distortions [8], in which case XYCORR produces a table of zeros or – as for spiral read-out imaging plate detectors – computes the small corrections resulting from radial (ROFF=) and tangential (TOFF=) offset errors of the scanner. For some multiwire- and CCD detectors that deliver geometrically distorted images, corrections are derived from a calibration image (BRASS_PLATE_IMAGE=file name). This image displays the response to a brass plate containing a regular grid of holes which is mounted in front of the detector and illuminated by an X-ray point source, e.g., ^{55}Fe. Clearly, the source must be placed exactly at the location to be occupied by the crystal during the actual data collection, as

photons emanating from the calibration source are meant to simulate all possible diffracted beam directions. For visual control using the VIEW program, spots that have been located and accepted from the brass plate image by XYCORR are marked in the file FRAME.pck.
Problems: (a) A misplaced calibration source leads to an incorrect lookup table, impairing the correct prediction of the observed diffraction pattern in subsequent program steps. (b) Underexposure of the calibration image results in an incomplete and unreliable list of calibration spots.

INIT estimates the initial background at each pixel and determines the trusted region of the detector surface. The total background at each pixel is the sum of detector noise and X-ray background. The detector noise, saved in the lookup table BLANK.TBL, is determined from a specific image recorded in the absence of X-rays (DARK_CURRENT_IMAGE=) or is assumed to be a constant derived from the mean recorded value in each corner of the data images. A lookup table of the X-ray background, saved on the file BKGINIT.pck, is obtained from the first few data images by the following two-pass procedure. To exclude diffraction spots in the data image, the minimum of the five values at $(x, y), (x \pm dx, y), (x, y \pm dy)$ is used as a lower background estimate at pixel (x, y) in the first pass. In the second pass, the background is taken as the maximum of the lower estimates at these five locations. Ideally, the parameters SPOT_WIDTH_ALONG_X=$2*dx+1$, SPOT_WIDTH_ALONG_Y=$2*dy+1$ are chosen to match the extent of a spot. The lookup table is obtained by adding the X-ray background from each image. Shaded regions on the detector (i.e., beam-stop) or pixels outside a user defined circular region (RMAX=) or pixels with an undefined spatial correction value are classified as untrustworthy and marked by -3. The table should be inspected using the VIEW program.
Problems: (a) The addition of background from too many data images may exceed 262,144 at some pixels which are removed from the trusted detector region due to internal number overflow. (b) Some detectors with insufficient protection from electromagnetic pulses may generate badly spoiled images whose inclusion leads to a completely wrong X-ray background table. These images can be identified in INIT.LP by their unexpected high mean pixel contents, and this step should be repeated with a different set of images.

COLSPOT locates, at most, 500,000 strong diffraction spots occurring in a subset of the data images and saves their centroids on the file SPOT.XDS. Up to ten ranges of contiguous images (SPOT_RANGE=) may be specified explicitly; otherwise, spots are taken from the first few data images, covering a total rotation range of 5°. Spots are located automatically by comparing each pixel value with the mean value and standard deviation of surrounding pixels. A lower threshold for accepting pixels and a minimum required number of such pixels within a spot can be defined in XDS.INP by the parameters
MINIMUM_SIGNAL_TO_NOISE_FOR_LOCATING_SPOTS= and
MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=, respectively.
Problems: (a) Sharp edges like ice rings in the images can lead to an excessive number of pixels erroneously classified as contributing to a diffraction spot which extends over many adjacent images, thereby causing a hash-table overflow. The problem can be avoided by specifying non-adjacent images for spot search.

IDXREF uses the initial parameters describing the diffraction experiment as provided by XDS.INP and the observed centroids of the spots occurring in the file SPOT.XDS to find the orientation, metric, and symmetry of the crystal lattice, and, it refines all or a specified subset of these parameters. On return, the complete set of parameters are saved in the file XPARM.XDS, and the original file SPOT.XDS is replaced by a file of identical name – now with indices attached to each observed spot. Spots not belonging to the crystal lattice are

given indices 0,0,0. XDS considers the run successful if at least 70% of the given spots can be explained with reasonable accuracy; otherwise, XDS will stop with an error message. Alien spots often arise because of the presence of ice or small satellite crystals, and continuation of data processing may still be meaningful. In this case, XDS is called again with an explicit list of the subsequent steps specified in XDS.INP.

Using and understanding the results reported in IDXREF.LP requires a knowledge of the concepts employed by this step, as described in reference [6]. First, a reciprocal lattice vector, referring to the unrotated crystal, is computed from each observed spot centroid. Differences between any two reciprocal lattice vectors which are above a specified minimal length (SEPMIN=) are accumulated in a 3-dimensional histogram. These difference vectors will form clusters in the histogram since there are many different pairs of reciprocal lattice vectors of nearly identical vector difference. The clusters are found as maxima in the smoothed histogram (CLUSTER_RADIUS=), and a basis of three linear independent cluster vectors is selected that allows all other cluster vectors to be expressed as nearly integral multiples of small magnitude with respect to this basis. The basis vectors and the 60 most populated clusters with attached indices are listed in IDXREF.LP. If many of the indices deviate significantly from integral values, the program is unable to find a reasonable lattice basis and all further processing will be meaningless.

If space-group and cell constants are specified, a reduced cell is derived, and the reciprocal basis vectors found above are reinterpreted accordingly; otherwise, a reduced cell is determined directly from the reciprocal basis. Parameters of the reduced cell, coordinates of the reciprocal basis vectors, and their indices with respect to the reduced cell are reported.

Based on the orientation and metric of the reduced cell now available, IDXREF indexes up to 3,000 of the strongest spots by the local indexing method. This method considers each spot as a node of a tree and identifies the largest subtree of nodes which can be assigned reliable indices. The number of reflections in the ten largest subtrees is reported and usually shows a dominant first tree corresponding to a single lattice, whereas alien spots are found in small subtrees. Reflections in the largest subtree are used for initial refinement of the basis vectors of the reduced cell, the incident beam wave vector, and the origin of the detector, which is the point in the detector plane nearest to the crystal. Experience has shown that the detector origin and the direction of the incident beam are often specified with insufficient accuracy, which could easily lead to a misindexing of the reflections by a constant offset. For this reason, IDXREF considers alternative choices for the index origin and reports their likelihood for being correct. Parameters controlling the local indexing are INDEX_ERROR=, INDEX_MAGNITUDE=, INDEX_QUALITY= (corresponding to ϵ, δ, $1 - \ell_{min}$ in reference [6], and INDEX_ORIGIN=h_0, k_0, l_0, which is added to the indices of all reflections in the tree. After initial refinement based on the reflections in the largest subtree, all spots which can now be indexed are included. Usually, detector distance and the direction of the rotation axis are not refined; but if the spots were extracted from images covering a large range of total crystal rotation, better results are obtained by including these parameters in the refinement (REFINE=).

The refined metric parameters of the reduced cell are used for testing each of the 44 possible lattice types, as described in reference [6]. For each lattice type IDXREF reports the likelihood of being correct, the conventional cell parameters, and the linear transformation relating original indices to the new indices with respect to the conventional cell. However, no automatic decisions for space-group assignment are made by XDS. If space-group and cell constants are provided by the user, the reduced cell vectors are reinterpreted accordingly; otherwise, data processing continues with the crystal being described by its reduced

cell basis vectors and triclinic symmetry. On completion, when integrated intensities are available, the user chooses any plausible space-group according to the rated list of the 44 possible lattice types and repeats only the CORRECT and GLOREF steps with the appropriate conventional cell parameters and reindexing transformation (see below).
Problems: (a)Indices of many difference vector clusters deviate significantly from integral values. This can be caused by incorrect input parameters, like rotation axis, oscillation angle, detector position, by a large fraction of alien spots in SPOT.XDS, by placing the detector too close to the crystal, or by inappropriate choice of parameters SEPMIN= and CLUSTER_RADIUS= in densely populated images. (b)Indexing and refinement is unsatisfactory despite well-indexed difference vector clusters. This is probably caused by selection of an incorrect index origin, and IDXREF should be rerun with plausible alternatives for INDEX_ORIGIN= after a visual check of a data image with the VIEW program.

DEFPIX defines the trusted region of the detector. It recognizes regions in the initial background table (file BKGINIT.pck) that are obscured by intruding hardware and marks the shaded pixels as untrusted. In addition, pixels outside a user-defined resolution range are marked and eliminated from the trusted region. The marked background table thus obtained is saved on file BKGPIX.pck which is needed by the subsequent program step.

COLPROF extracts the three-dimensional profile of each reflection predicted to occur in the rotation images within the trusted region of the detector surface and saves all profiles on the file XREC.XDS. A scaling factor is determined for each image, derived by comparing its background region (after subtraction of the detector noise) with the current X-ray background table. This table, initially obtained from the file BKGPIX.pck, is updated by the background from each data image at a rate defined by the input parameter BFRAC=. For visual control, the contents of the updated X-ray background table is saved on the file BKGfinal.pck at the end of this program step. Information for predicting reflection positions is initially provided by the file XPARM.XDS. These parameters are either kept constant or refined periodically using centroids of the most recently found strong diffraction spots as data reduction proceeds (REFINE=, NUMBER_OF_FRAMES_BETWEEN_REFINEMENT_IN_COLPROF=,
NUMBER_OF_REFLECTIONS_USED_FOR_REFINEMENT_IN_COLPROF=, WEAK=).

In order to include all pixels contributing to the intensity of a spot, approximate values describing their extension and form must be specified. A value for BEAM_DIVERGENCE= arctan(spot diameter/detector distance) is found by measuring the diameter of a strong spot in a data image displayed by the VIEW program and should include a few adjacent background pixels. The form of a spot is roughly described as a Gaussian and its standard deviation is specified by the parameter BEAM_DIVERGENCE_E.S.D.=, which is usually about 1/6 to 1/10 of BEAM_DIVERGENCE=. Similarly, REFLECTING_RANGE= is the approximate rotation angle required for a strong spot recorded perpendicular to the rotation axis to pass completely through the Ewald sphere. The standard deviation of the intensity distribution is given by the mosaicity (REFLECTING_RANGE_E.S.D.=σ_M). Thus, a three-dimensional domain of pixels belonging to each reflection is defined by the above parameters, and the program automatically removes pixels contaminated by neighbouring reflections. It determines and subtracts the background, corrects for spatial distortions, and maps each pixel content into a reflection-specific coordinate system centered on the Ewald sphere [5]. The form of these profiles is then similar for all reflections, and their mean obtained from superimposition of strong reflections is reported at regular intervals. On return from this step, the data image last processed with all expected spots encircled is saved in the file FRAME.pck for inspection using the VIEW program.

Problems: (a) Off-centered profiles indicate incorrectly predicted reflection positions by using the parameters provided by the file XPARM.XDS (i.e., misindexing by using a wrong origin of the indices), crystal slippage, or change in the incident beam direction. (b) Profiles extending to the borders of the box indicate too-small values for BEAM_DIVERGENCE= or REFLECTING_RANGE=. This leads to incorrect integrated intensities because of truncated reflection profiles and unreliable background determination. (c) Display of the file FRAME.pck showing spots which are not encircled. If these unexpected reflections are not close to the spindle and are not ice reflections, it is likely that the parameters provided by the file XPARM.XDS are wrong.

PROFIT estimates intensities from the three-dimensional profiles of the reflections stored in the input file XREC.XDS and saves the results on the file PROFIT.HKL. In the first pass, templates are generated by superimposing profiles of fully recorded, strong reflections, and all grid points with a value above a minimum percentage of the maximum in the template (CUT=) are defined as elements of the integration domain. To allow for variations of their shape, profile templates are generated from reflections located at nine regions of equal size covering the detector surface and additional sets of nine to cover equally-sized batches of images. Standard deviations, REFLECTING_RANGE_E.S.D.= and BEAM_DIVERGENCE_E.S.D.=, observed for each profile template are reported and – in case of large discrepancies – could be used for rerunning COLPROF with better values for these parameters. In the second pass, intensities and their standard deviations are estimated by fitting the reflection profile to its template, as described in reference [5]. Overloaded (OVERLOAD=) or incomplete reflections covering less than a minimum percentage of the template volume (MINPK=) or reflections with unreliable background are excluded from further processing.
Problems: (a) The program stops because there are no strong spots for learning profile templates. It is likely that, parameters REFLECTING_RANGE=,
BEAM_DIVERGENCE=, etc., which define the box dimensions have been incorrectly chosen. After correction, both the COLPROF and PROFIT step should be repeated.

CORRECT applies Lorentz- and polarization correction factors as well as factors which partially compensate for radiation damage and absorption effects to intensities and standard deviations of all reflections found in the file PROFIT.HKL and saves the results on the file XDS_ASCII.HKL. These factors are determined from many symmetry-equivalent reflections usually found in the data images such that their integrated intensities become as similar as possible. The residual scatter of these intensities is a more realistic measure of their errors and used to determine a correction factor for the standard deviations previously estimated from profile fitting. Based on the more realistic error estimates of the intensities, outliers are recognized by comparison with other symmetry-equivalent reflections. These outliers are included in the main output file XDS_ASCII.HKL in which they are marked by a negative sign attached to the estimated standard deviations of their intensity. Classification of a reflection as a misfit is controlled by a decision constant which has the default value of WFAC1=1.5. A lower value (i.e. WFAC1=1.0) specified by the user will lead to an increasing number of misfits and lower R-factors as outliers are not included in the reported statics.

Data quality as a function of resolution is described by the agreement of intensities of symmetry-related reflections and quantified by the R-factors, R_{sym}, and the more robust indicator, R_{meas} [2]. These R-factors as well as the intensities of all reflections with indices of type $h00$, $0k0$, and $00l$ and those expected to be systematically absent are important indicators for identification of the correct space-group. Clearly, large R-factors or many rejected

reflections (MISFITS) or large observed intensities for systematically absent reflections suggest that the assumed space-group or the indexing is incorrect. It is easy to test other possible space-groups (SPACE_GROUP_NUMBER=) by simply repeating the CORRECT and GLOREF steps after copying the appropriate reindexing transformation (REIDX=) and conventional cell constants (UNIT_CELL_CONSTANTS=) found in the rated table of the 44 possible lattice types in IDXREF.LP to XDS.INP. One should remember, however, that the final choice to be kept should be run last, as XDS overwrites earlier versions of the output files.

Another useful feature is the possibility to compare the new data with those from a previously measured crystal (REFERENCE_DATA_SET=file name). For some space-groups, like $P4_2$, possessing an ambiguity in the choice of axes, comparison with the reference data set allows one to identify the consistent solution from the complete set of alternatives already listed in IDXREF.LP together with their required index transformation. Reference data are also found quite useful for recognizing misindexing or for testing potential heavy-atom derivatives.
Problems: (a) Incomplete data sets may lead to wrong conclusions about the space-group, as some of its symmetry operators might not be involved in the R-factor calculations. (b)Conventional cell parameters, as listed in IDXREF.LP, often violate constraints imposed by the space-group and must be edited accordingly after copying to XDS.INP.

GLOREF refines the diffraction parameters by using the observed positions of all strong spots contained in the file PROFIT.HKL. It reports the root-mean-square error between calculated and observed positions along with the refined unit cell constants. Again, for testing possible space-groups, the crystallographer consults the table printed by the IDXREF step and selects the appropriate reindexing transformation and starting values for the conventional cell constants. The refined diffraction parameters (after possible reindexing) are saved on the file GXPARM.XDS, which is identical in format to XPARM.XDS. Replacing XPARM.XDS with the new file offers a convenient way for repeating COLPROF, now with a better set of parameters.
Problems: (a) GLOREF will fail if the crystal slips during data collection.

2.3 XPLAN

XPLAN supports the planning of data collection. It is based upon information provided by XPLAN.INP and the input files XPARM.XDS, BKGPIX.pck, both of which are available by processing a few test images with XDS. XPLAN estimates the completeness of new reflection data, expected to be collected for each given starting angle and total crystal rotation, and reports the results for a number of selected resolution shells in the file XPLAN.LP. To minimize recollection of data, the name of a file containing already measured reflections can be specified in XPLAN.INP.
Problems: (a)Incorrect results may occur for some space-groups, i.e., $P4_2$, if the unit cell determined by XDS from processing a few test images implicates reflection indices inconsistent with those from the already measured data. The correct cell choice can be found, however, by using the old data as a reference and repeating CORRECT and GLOREF with the appropriate reindexing transformation, followed by copying GXPARM.XDS to XPARM.XDS. The same applies if IDXREF was run for an unknown space-group and then reindexed in CORRECT and GLOREF. (b)XPLAN ignores potential reflection overlap due to the finite oscillation range covered by each image.

2.4 XSCALE

XSCALE accepts one or more files of type XDS_ASCII (or the old file types DIRECT ANOMAL NORMAL UNIQUE) obtained from data processing with XDS, determines scaling factors for the reflection intensities, optionally merges symmetry-equivalent observations into a unique set (MERGE=TRUE—FALSE), and reports data completeness and quality on the file XSCALE.LP. Misfits (recognized by a negative $\sigma(I)$) as well as reflections that should be systematically absent are ignored in the input files. XSCALE also allows to generate separate output files, each comprising one or several input data sets, that are on a common scale - a useful feature for MAD data sets.

The desired program action is specified in the file XSCALE.INP. This file contains the parameter values that define resolution shells used for reporting data quality and completeness, space-group number and cell constants, as well as the names and associated information of the input and output reflection files.
Problems: (a)All reflections beyond the highest shell specified for analyzing resolution dependency of data quality and completeness will be ignored regardless of the resolution window given for each data set.

2.5 VIEW

VIEW is used for visualizing data images as well as control images produced by XDS. It responds to navigation commands entered by movements of a mouse and reports the corresponding image coordinates and their pixel content upon activation of the mouse-buttons. VIEW also allows magnification of selected image portions and change in color.
Problems: (a) For many detector image formats as well as XDS produced images, the true pixel value is stored in a coded form which is interpreted by VIEW as a signed integer. Numbers less than -4095 displayed by VIEW correspond to large positive pixel values.

2.6 XDSCONV

XDSCONV accepts reflection intensity data files as produced by XSCALE or CORRECT and converts them into a format required by software packages for structure determination. For use by the SHELX [7] program, scaled intensity data are (optionally) provided prior to merging symmetry equivalent reflections and XDSCONV only reformats the reflection records. For other packages like CNS [1], XDSCONV estimates structure factor moduli based on the assumption that the intensity data set obeys Wilson's [9] distribution. It uses a Bayesian approach to statistical inference as described by French and Wilson [3].

XDSCONV has the capability to inherit the indices of test-reflections previously used for the calculation of the free R-factor, and to select new test-reflections that are outside the resolution range covered by the inherited test-reflections. This extension of the test-set is required if new data at a higher resolution become available that should be included in the structure refinement process.

3 Remarks

XDS is not an interactive program. It communicates with the input file XDS.INP and during the run accepts only a change in specification of the last image to be included in the data

set (DATA_RANGE=) – a useful option when processing overlaps with data collection. To prevent the program from overtaking the measurements, a maximum delay should be set (MINUTE=) to be slightly longer than the time for generating the next image.

Experience has shown that the most frequent obstacle in using the package is the indexing and accurate prediction of the reflections occurring in the images. Usually, the problems arise from incorrect specifications of rotation axis, beam direction, detector position, and orientation, oscillation range, or wavelength. The occurrence of gross errors can be reduced by using file templates of XDS.INP specifically tailored to the actual experimental set-up which require only small adjustments to the geometrical parameters.

Still, even small errors in the specification of the incident beam direction or the detector position may lead to indices which are all offset by one reciprocal lattice point, particularly if the initial list of diffraction spots was obtained from a few images covering a small range of crystal rotation. For this reason, IDXREF tests a few alternatives for the index origin and reports its results, such as the expected coordinates of the incident beam in the image, which can be checked by looking at a data image with the VIEW program. The user may then repeat the IDXREF step, thereby forcing the program to use a plausible alternative for the index origin.

It is recommended to run all program steps on a few images to establish whether the indexing is correct and also to find reasonable values describing crystal mosaicity and spot size. Incorrect indexing may be apparent from large values of symmetry R-factors or from comparison with a reference data set reported in the CORRECT step. Also, looking at the file FRAME.pck with the VIEW program should show the last data image processed with most of the observed diffraction spots circled. More accurate estimates of the parameters describing spot dimensions are reported in PROFIT.LP and should be used for updating these values in XDS.INP before starting data processing for all images.

Refinement of parameters controlling the predicted position of spots are carried out in the IDXREF, COLPROF, and GLOREF step, which allows the user to adopt a variety of strategies. If all data images are available, spots should be extracted by COLSPOT from images equally distributed in the data set. If IDXREF is able to explain most of the spots, the refined parameters will be sufficiently accurate for the complete data processing, and refinements in the COLPROF step are unnecessary. In other cases, if processing overlaps with data collection or the first strategy was unsuccessful, IDXREF is based on spots extracted from the first few images and provides an initial parameter set which is periodically refined during COLPROF. This allows correction for slow crystal slippage or minor changes of the incident beam direction. Finally, if refinement in GLOREF was successful, the new values may be used to repeat COLPROF (without parameter refinements) and subsequent steps.

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TABLE 1 Information exchange between program steps of XDS

program step	input files		output files	
	name	type	name	type
XYCORR	XDS.INP	ASCII	XYCORR.LP	ASCII
			XYCORR.TBL	DIR
			FRAME.pck	BIN
INIT	XDS.INP	ASCII	INIT.LP	ASCII
	XYCORR.TBL	DIR	BKGINIT.pck	BIN
			BLANK.TBL	DIR
COLSPOT	XDS.INP	ASCII	COLSPOT.LP	ASCII
	BKGINIT.pck	BIN	SPOT.XDS	ASCII
	BLANK.TBL	DIR	FRAME.pck	BIN
	XYCORR.TBL	DIR		
IDXREF	XDS.INP	ASCII	IDXREF.LP	ASCII
	SPOT.XDS	ASCII	SPOT.XDS	ASCII
			XPARM.XDS	ASCII
DEFPIX	XDS.INP	ASCII	DEFPIX.LP	ASCII
	XPARM.XDS	ASCII	BKGPIX.pck	BIN
	BKGINIT.pck	BIN	ABS.pck	BIN
	XYCORR.TBL	DIR		
COLPROF	XDS.INP	ASCII	COLPROF.LP	ASCII
	XPARM.XDS	ASCII	XREC.XDS	BIN
	BKGPIX.pck	BIN	BKGfinal.pck	BIN
	BLANK.TBL	DIR	FRAME.pck	BIN
	XYCORR.TBL	DIR		
PROFIT	XDS.INP	ASCII	PROFIT.LP	ASCII
	XREC.XDS	BIN	PROFIT.HKL	DIR
CORRECT	XDS.INP	ASCII	CORRECT.LP	ASCII
	PROFIT.HKL	DIR	XDS_ASCII.HKL	ASCII
GLOREF	XDS.INP	ASCII	GLOREF.LP	ASCII
	PROFIT.HKL	DIR	GXPARM.XDS	ASCII